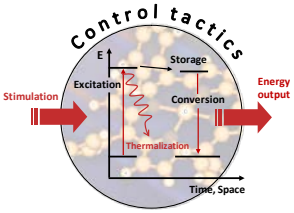

Computational insights into the reactivity of molecular inorganic catalysts in solution

Ricardo A. Mata
Institute of Physical Chemistry
Georg-August University Göttingen

Solvation plays a fundamental role in chemistry, strongly influencing catalysis in biological systems and industrial processes. A reaction can be stopped or accelerated several orders of magnitude depending on the choice of solvent. The theoretical modeling of these effects has led to a zoo of different methods, each with different complexity and application range. In this talk, we discuss recent developments made in our group towards the computational treatment of reactivity in solution, through the use of both explicit (Monte Carlo QM/MM approaches) and implicit (continuum model) solvation schemes.
Applications in molecular inorganic complexes will be discussed, including redox reactions in Mo enzymes as well as a few selected examples on synthesized compounds. We show that through a consistent treatment of solvation and the overall chemical environment, it is possible not only to tap into new reaction pathways but also correctly evaluate the energetics of these processes.